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# Free motion time-of-arrival operator and probability distribution

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We reappraise and clarify the contradictory statements found in the literature concerning the time-of-arrival operator introduced by Aharonov and Bohm in Phys. Rev. **122**, 1649 (1961). We use Naimark's dilation theorem to reproduce the generalized decomposition of unity (or POVM) from any self-adjoint extension of the operator, emphasizing a natural one, which arises from the analogy with the momentum operator on the half-line. General time operators are set within a unifying perspective. It is shown that they are not in general related to the time of arrival, even though they may have the same form.

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## I. INTRODUCTION

Even though there is no question that experimentalists measure distributions of time of arrival for quantum systems, there has been a long debate about the capabilities of standard quantum mechanics to address the very concept of time as an observable. In a nutshell, the problem arises because we expect observables to be represented in the quantum formalism by self-adjoint operators, whereas an old theorem of Pauli [1] states that for a semibounded self-adjoint operator  $\hat{H}$  no conjugate self-adjoint operator  $\hat{T}$  can exist, i.e., no operator that is self-adjoint and satisfies the canonical commutation relation  $[\hat{H}, \hat{T}] = i\hbar$  over a dense domain. In other words, there is no self-adjoint time operator if the Hamiltonian is bounded from below, as we normally expect it to be. However the theorem has not discouraged theorists from attempting to fit such an immediate classical concept into the standard framework (see [2] for a general discussion). In relatively recent times a rather satisfactory answer has been given for the arrival time of freely moving states in one dimension, from the point of view of generalized spectral functions, or positive-operator-valued measures (POVM) [3–6]. In short, the relevant statement is that self-adjointness is not strictly necessary for the formulation of probabilities and the reality of measurements of observables, and that, in fact, any given observable is uniquely characterized (in a specific sense) by the probability distributions of measurement results in the different states accessible to the system (for a much more developed presentation, refer to [4,5]).

This result has sparked a renewed interest in the analysis of old and new proposals for time operators in general, and in particular for the time-of-arrival operator  $\hat{T}_{AB}$  (see below) introduced by Aharonov and Bohm [7], as in [6,8–21].

However, a number of basic issues are still in dispute, or in need of clarification. In particular, contradictory statements may be found about the domain of the time

operator  $\hat{T}_{AB}$  [9,14], or about its eigenfunctions [16,14]; and the deficiency indices, which are important to determine its self-adjoint extensions, appear to be, following different authors, either (0,1) or (0,2) [10,14], but only one of the possibilities may be correct. Even though several self-adjoint “variants” of  $\hat{T}_{AB}$  have been proposed, [11,16,15] none of them is a self-adjoint extension of  $\hat{T}_{AB}$  in a proper sense. The framework to consider these extensions is Naimark's dilation theorem [4,5,22], but an explicit simple construction of a self-adjoint extension is lacking (For a rather abstract presentation of the theorem applied to the time-of-arrival problem, under the guise of “screen observables”, see [13]; also [4,6,5]). In addition, the form of the time operators in different representations may also be, and has been, misleading: the same operator has been presented in different forms, but different operators have also been written in the same form.

It appears that in order to make further progress in this field without being trapped by any of the numerous pitfalls mentioned, a detailed analysis of these topics is required, and their clarification is the main objective of this paper. Even though some of the arguments have to be rather technical, our aim is to provide an account readable by a general physicist. We shall in particular introduce a description of the extension theorems as they apply to the problem at hand, and develop a general analogy, sketched by Holevo [4], between the momentum operator in the half line and the time operator. We hope that it will provide a much better understanding of the relevant issues. It will also allow to join the strands given by i) the initial proposal of the time-of-arrival operator of Aharonov and Bohm [7], its modifications or variants [11,15–17]; ii) the POVM idea as applied to quantum physics and to the time operator in particular [5,14]; iii) the axiomatic approach of Kijowski to obtain good probability distributions for the time of arrival [11,12]; and iv) some apparently formal constructions in Allcock's seminal paper [8].

As is well known, the momentum operator in the half-line is not self-adjoint. Moreover, it is maximally symmetric, because its deficiency indices are  $(1, 0)$ , and it admits no self-adjoint extension on the Hilbert space of functions defined on the half-line (for a fast and good review of deficiency indices and the Neumann theory of extensions, with particular emphasis on the physical examples of momentum operator and Laplacian, see [23] - we will anyhow give a self-contained description in section II). On the other hand, there is a natural extension, namely, the momentum operator on the full line. It should be noticed that this is most definitely not the unique extension, but just one of the infinitely many possible. Nonetheless, its “naturalness” is well justified from a physical point of view. The question might then be posed as to how are we to recover any information about the distribution of probability of momentum in the half-line from the full line extension. This is actually the content of Naimark’s dilation theorem, together with the theorem that asserts the uniqueness of the POVM associated with a maximally symmetric operator: that the *unique* distribution of probability associated with the momentum operator on the half-line is recovered from the spectral decomposition of the self-adjoint operator momentum on the full line, by simple projection. Equivalently stated, we can reproduce the *physical* content of the momentum operator on the half-line from the standard, well-known techniques that apply to self-adjoint operators.

We will show that the different alternatives that have been proposed to make sense of the time operator of Aharonov and Bohm are actually consequences of this general result, that we have phrased in terms of momentum operators, but which can be extended to other cases as well. The generality of the result also explains the coincidence of different constructions, in particular the axiomatic approach of Kijowski [11,12] and the attempts to create ex novo a self-adjoint operator ([15] is a relevant example).

We organize the paper as follows: in the next section we give a complete and very basic description of the momentum operator on the half-line and the problems that appear there. We also give the natural extension and describe more fully Naimark’s dilation theorem in this context. In section III we establish the parallel with the time-of-arrival operator of Aharonov and Bohm, to be followed in the next section with the general case of a time operator. Section V is devoted to discussing and restating the different results known in the literature in the terms used in the previous sections.

## II. THE MOMENTUM OPERATOR

Consider the momentum operator  $\hat{p} = -i\hbar\partial_x$  defined on a dense domain of the Hilbert space of square integrable functions on the half-line,  $\mathcal{H}_> = L^2(\mathbf{R}^+, dx)$ .

More precisely, it is defined on  $D(\hat{p})$ , the subspace of square integrable absolutely continuous functions  $\psi$  whose derivative is also square integrable, and such that  $\psi(0) = 0$ . Clearly, this operator is symmetric on its domain. Let us write down a set of generalized (weak) eigenfunctions that provide us with a resolution of the identity. The adequate set, which does not belong to the Hilbert space and is parametrized by real  $p$ , is given by  $\psi_p(x) = \exp(ipx/\hbar)/\sqrt{2\pi\hbar}$ , as is only to be expected. They form a complete basis, since  $\int_{-\infty}^{\infty} dp \overline{\psi_p(x')} \psi_p(x) = \delta(x' - x)$ . However, they are not orthogonal (in the generalized sense):

$$\int_0^{\infty} dx \overline{\psi_{p'}(x)} \psi_p(x) = \frac{1}{2} \delta(p - p') + \frac{i}{2\pi} \text{P} \frac{1}{p - p'},$$

where P stands for principal part. This is evidently different from the usual constructions for self-adjoint operators.

Let us now pass on to the position operator  $\hat{x}$ , defined on those square integrable functions on the half-line,  $\psi \in \mathcal{H}_>$ , such that  $\int_0^{\infty} dx x^2 |\psi(x)|^2 < +\infty$ . This operator is self-adjoint on its domain. Additionally, it is true that  $[\hat{x}, \hat{p}] = i\hbar$  on a dense domain. However, in the case at hand the position operator is bounded from below, and Pauli’s theorem therefore applies. It follows that  $\hat{p}$  is not a self-adjoint operator and admits no self-adjoint extension in  $\mathcal{H}_>$ .

We shall now rephrase the statements of the previous two paragraphs in a different way. The domain of the operator adjoint to  $\hat{p}$ , i.e.,  $\hat{p}^\dagger$ , according to von Neumann’s formula, is  $D(\hat{p}) \oplus N(i) \oplus N(-i)$ , where  $N(\pm i)$  are the spaces of eigenvectors of  $\hat{p}^\dagger$  with eigenvalues  $\pm i$  respectively. This comes about because, even though  $\hat{p}$ , being symmetric, has no imaginary eigenvalues, its adjoint does have eigenvectors with imaginary eigenvalues. As a matter of fact, the functions  $\exp(i\lambda x/\hbar)$ , with  $\lambda$  a complex number with positive imaginary part, are all of them eigenvectors of  $\hat{p}^\dagger$  of eigenvalue  $\lambda$ . Notice that the dimension of  $N(\lambda)$ , the space of eigenvectors with eigenvalue  $\lambda$ , is the same for all  $\lambda$  with positive imaginary part. This is called the first deficiency index of the operator  $\hat{p}$ , while the second one is the dimension of the space of eigenvectors for any given eigenvalue of negative imaginary part, in our case, 0. That is, the deficiency indices of  $\hat{p}$  are  $(1, 0)$ . But self-adjoint operators have deficiency indices  $(0, 0)$ , as do essentially self-adjoint operators, which, although not self-adjoint, have a unique self-adjoint extension, namely, their closure. If we were to build a self-adjoint extension of  $\hat{p}$  we would need to include somehow those elements of  $D(\hat{p}^\dagger)$  that are not in  $D(\hat{p})$ , but in such a way that the imaginary parts compensate. When the deficiency indices are equal, this is achieved by the use of a unitary transformation from  $N(\bar{\lambda})$  to  $N(\lambda)$  (this is the von Neumann theory of self-adjoint extensions, whereby each self-adjoint extension in the Hilbert space of definition of an operator over a dense domain, with equal defect indices, is given by a unitary transformation be-

tween the deficiency subspaces). As the deficiency indices in our case are different, it is not possible to extend  $\hat{p}$  to include an action over the whole of the domain of  $D(\hat{p}^\dagger)$  such that the imaginary parts compensate. Since  $\hat{p}$  is a closed operator, symmetric over its domain, which is dense in  $\mathcal{H}_>$ , and its deficiency indices are unequal, one of them being 0, we say that it is a maximally symmetric operator, and the previous result is that it admits no self-adjoint extension over  $\mathcal{H}_>$ .

Retaking the complete set of generalized eigenfunctions  $\psi_p(x)$ , we can construct a positive-operator-valued measure (POVM)  $F$ . This is a map from intervals in the real line (a  $\sigma$ -algebra of subsets of a nonempty set) to the positive operators over a Hilbert space that satisfies three axioms that we will illustrate with the example at hand. The map for our case is given by

$$\langle \phi | F([a, b]) \psi \rangle = \int_a^b dp \int_0^\infty dx \int_0^\infty dy \overline{\phi(x)} \psi_p(x) \overline{\psi_p(y)} \psi(y),$$

over all  $\phi, \psi \in \mathcal{H}_>$ . This map sends intervals of the real line to positive operators acting on  $\mathcal{H}_>$  (first axiom), which add together when the intervals are disjoint (second axiom), and which add to the identity operator when summed over the real line, because of the completeness proved above (third axiom). This differs from the usual decompositions for self-adjoint operators in that it does not fulfill the property that the positive operators be projectors, i.e., in our case  $F([a, b])^2 \neq F([a, b])$ , because of the lack of orthogonality shown above.

Now we have the POVM associated with  $\hat{p}$ , we can reconstruct the operator and the probability distribution of its values. The action of the operator is given by

$$(\hat{p}\varphi)(x) = \int_{-\infty}^\infty dp \int_0^\infty dy p \psi_p(x) \overline{\psi_p(y)} \varphi(y).$$

The probability distribution for its possible values over a state  $\psi$  is

$$\Pi_\psi(p) = \left| \int_0^\infty dx \overline{\psi_p(x)} \psi(x) \right|^2.$$

Notice that this indeed satisfies all the requirements for it to be a probability.

Let us see in more detail the relationship between the probability density and the POVM. We have written above the expression for the action of  $F([a, b])$ . Symbolically, we can write  $F(dp)$ , and its expectation value on a state  $\psi$  is

$$\begin{aligned} \langle \psi | F(dp) \psi \rangle &= \int_0^\infty dx \int_0^\infty dy \overline{\psi_p(x)} \frac{e^{ip(x-y)/\hbar}}{2\pi\hbar} \psi(y) dp \\ &= \Pi_\psi(p) dp. \end{aligned}$$

The expression just written defines in fact  $\langle \phi | F(dp) \psi \rangle$ , and therefore the whole POVM. Furthermore, the domain of the operator associated with the POVM is also

defined by  $\Pi_\psi(p)$ : by integration by parts it can readily be seen that the domain of the operator  $\hat{p}$  is precisely the set of states  $\psi$  for which the second moment of the probability distribution  $\Pi_\psi(p)$  is finite, and there it coincides with  $\|\hat{p}\psi\|^2$ . Therefore, the probability density written above defines the POVM and the operator with it associated. Notice also that the probability density need not be a continuous function. The only requirement is that  $\Pi_\psi(p)dp$  be a good measure on the real line.

Another important property of the POVM is covariance under displacements of momenta, which reflects the commutation relation  $[\hat{x}, \hat{p}] = i\hbar$ . Namely, it is readily computed that, for all real  $q$ ,

$$\langle \phi | e^{iq\hat{x}/\hbar} F([a, b]) e^{-iq\hat{x}/\hbar} \psi \rangle = \langle \phi | F([a + q, b + q]) \psi \rangle.$$

In terms of the probability density, the statement is that

$$\Pi_{\psi_q}(p) = \Pi_\psi(p + q),$$

where  $\psi_q = e^{-iq\hat{x}/\hbar} \psi$  is the shifted state.

The probability density, written above for the case of pure states, can be easily generalized to mixed states. Let  $\rho(y, x)$  be the matrix elements of the density matrix  $\hat{\rho}$  in the position representation. The probability density associated with this density matrix is then

$$\Pi_\rho(p) = \int_0^\infty dx \int_0^\infty dy \frac{e^{ip(x-y)/\hbar}}{2\pi\hbar} \rho(y, x).$$

In what follows we will use only pure states in the discussion, bearing in mind that the generalization to mixed states is straightforward.

It would seem that something akin to the spectral theorem of self-adjoint operators has been achieved, and this is indeed the case. The difference, however, lies in that the expectation value of higher order powers of  $\hat{p}$  on a state  $\psi$ ,  $\langle \psi, \hat{p}^n \psi \rangle$ , does not necessarily coincide with the corresponding moment of the distribution  $\Pi_\psi(p)$ , i.e.,  $\int_{-\infty}^\infty dp p^n \Pi_\psi(p)$ , for  $n \geq 3$ . For the case at hand, for instance, this happens already for  $n = 3$  if  $\psi'(0) \neq 0$ . As a matter of fact, in such a situation the expectation value for  $\hat{p}^3$  has an imaginary part. Nonetheless, the measures of momenta can be readily associated with  $\Pi_\psi(p)$ , which carries the relevant physical information.

Even so, we would normally like to understand the constructions above in terms of the more usual recipes for self-adjoint operators. We shall now make essential use of the uniqueness theorem for POVMs of maximally symmetric operators: given a maximally symmetric operator  $\hat{A}$  over a Hilbert space  $\mathcal{H}$ , there is a unique POVM,  $F_A$  (unique up to isomorphisms), such that its first operator moment coincides with the operator, and that the set of states over which the second moment exists is precisely the domain of  $\hat{A}$  [5,22]. This means that if we are to construct by whichever means a POVM such that it fulfills these conditions, we will be obtaining again the same POVM.

Moreover, Naimark's dilation theorem tells us that any POVM associated with a symmetric operator defined on a dense subset of  $\mathcal{H}$  can be constructed from a self-adjoint extension of the operator to a larger space  $\tilde{\mathcal{H}}$ , as follows: let  $E$  be the projection valued measure of the self-adjoint extension (i.e., a POVM that satisfies the further requirement that  $E([a, b])^2 = E([a, b])$ ), and  $P$  the projection operator from  $\tilde{\mathcal{H}}$  to  $\mathcal{H}$ . Then  $F([a, b]) := PE([a, b])$  is a POVM associated with the symmetric operator.

As a consequence, if we are to build a self-adjoint extension of  $\hat{p}$  in a larger space, we reproduce the unique POVM and the whole of the physical content of the operator from the usual analysis for the self-adjoint extension and a projection. Notice however that the possible extensions are infinite. Not so the POVM, and that makes the freedom of choice of extension even more interesting.

Back to the case of  $\hat{p} = -i\hbar\partial_x$  defined on the half-line, we see that there is a simple possibility: to extend the operator to the full line, i.e.,  $-i\hbar\partial_x$  defined on a dense subset of  $\mathcal{H} = L^2(\mathbf{R}, dx)$ . Naturally enough, the action of this operator on the elements of  $D(\hat{p})$  is the same as that of  $\hat{p}$ , so it is an extension. This is not the only self-adjoint extension on the whole real line, of course. As a matter of fact, the deficiency indices for the direct sum of the momentum operators on the positive and negative half-lines are  $(1, 1)$ , thus signalling that a one dimensional continuum of alternative self-adjoint extensions exist. They differ by the presence of a jump function located on  $x = 0$ . However, most natural is the momentum on the full line, defined over absolutely continuous functions, i.e. with no jump on  $x = 0$ . This is a self-adjoint operator, for which the standard spectral analysis is applicable.

More concretely, the projection valued measure  $E$  is given by the expression

$$\langle \phi | E([a, b]) \psi \rangle = \int_a^b dp \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \overline{\psi_p(y)} \psi_p(x) \overline{\phi(x)} \psi(y),$$

with  $\psi_p(x) = \exp(ipx/\hbar)/\sqrt{2\pi\hbar}$ , as before, but now defined over the whole real line. The projection  $P$  in our case is simply  $(P\psi)(x) = \Theta(x)\psi(x)$ , with  $\Theta$  being Heaviside's step function.

The probability distribution for the momentum operator over the whole real line for a state  $\psi$  is of course the modulus squared of the wave function in the momentum representation, and its restriction to states that belong to  $D(\hat{p})$  is none other than the probability distribution associated with the POVM.

We see then that the reason we could not do the standard analysis for the momentum operator on the half-line is that we are being, in a way, far too restrictive in the behaviour near  $x = 0$  of the states on which it can act. There is a reminder of the full line, seen for instance in the principal part that forbids orthogonality, or in the fact that the higher moments of the probability distribution do not in general agree with the expectation value of powers of the restricted momentum operator. If our

states were such that the function  $\psi$  and all of its derivatives were zero at  $x = 0$ , there would be no problem with the higher moments, and we would get no imaginary part for the powers of  $\hat{p}$  over such states. However, such a strong restriction on the allowable wavefunctions would cut out many physically sensible cases.

Let us now write slightly more formally the extension procedure we have performed to reobtain and interpret the probability density: we have started with a maximally symmetric operator  $\hat{p} = -i\hbar\partial_x$  acting on the dense domain  $D(\hat{p}) \subset \mathcal{H}_> = L^2(\mathbf{R}^+, dx)$ , with deficiency indices  $(1, 0)$ . We have then considered an extension in  $L^2(\mathbf{R}, dx)$ , making use of the isomorphism

$$L^2(\mathbf{R}, dx) = L^2(\mathbf{R}^+, dx) \oplus L^2(\mathbf{R}^-, dx).$$

The extension has been the natural one, i.e.,  $-i\hbar\partial_x$  on the full line (although, as we repeatedly stated, this is not the only possible extension; another easy choice would have been some extension of  $\hat{p} \oplus (-\hat{p})$ , for instance). The standard spectral analysis for this operator produces the probability density, which, when restricted to  $\mathcal{H}_>$ , gives  $\Pi_\psi(p)$ , the probability density out of which the POVM for the operator we started from can be built.

### III. THE TIME-OF-ARRIVAL OPERATOR

Within the long-running discussion on the concept of time in quantum mechanics, and in particular with respect to the status of the time-energy uncertainty relations, Aharonov and Bohm introduced in an important paper [7], among other questions, "a clock" to measure time from the position and momentum of a freely moving test particle. The corresponding operator was obtained by a simple symmetrization of the classical expression  $my/p_y$ , where  $y$  and  $p_y$  are, respectively, the position and momentum of the test particle. By the same token, the operator obtained by symmetrizing the classical expression for the arrival time at  $x = 0$  of a freely moving particle having position  $x$  and momentum  $p$ ,  $t = -mx/p$ , is given by [2,20]

$$\hat{T}_{AB} := -\frac{m}{2} (\hat{x}\hat{p}^{-1} + \hat{p}^{-1}\hat{x}),$$

Note the minus sign in comparison to the clock time in [7]. In spite of the somewhat subtle difference (in concept and sign) with the original time operator introduced in [7] we shall refer to this operator as the Aharonov-Bohm (time-of-arrival) operator. Without regard for topological considerations, it is clear that it has the correct commutation relation with the free particle Hamiltonian on the line,  $\hat{H}_0 = \hat{p}^2/2m$ . It is thus a good candidate for a time operator, with the plausible physical interpretation, given by the correspondence rule, that it is related to the time of arrival (notice that other quantization rules might possibly give a different result, although this is the operator obtained not just by the symmetrization

rule, but also by applying Weyl, Rivier, or Born-Jordan quantizations [24]). However, it also follows, from Pauli's theorem, that it cannot be a self-adjoint operator acting on a dense space.

Let us then examine first the question of the domain of  $\hat{T}_{AB}$ . In order to do that, it is useful at this point to consider the Hilbert space of the free particle in the momentum representation,  $\mathcal{H}_p := L^2(\mathbf{R}, dp)$  (on this space we know how  $\hat{p}^{-1}$  acts, thanks to the spectral theorem). Formally, we then obtain

$$\hat{T}_{AB} \rightarrow \frac{i\hbar m}{2} \left( \frac{1}{p^2} - \frac{2}{p} \frac{\partial}{\partial p} \right).$$

There are other alternative expressions, such as  $-i\hbar m p^{-1/2} \partial_p p^{-1/2}$ , which would be valid for  $p > 0$ , or for  $p < 0$  by analytic continuation, see e.g. [16]. At any rate,  $\hat{T}_{AB}$  understood as a differential operator presents a singular point at  $p = 0$ , and this is the source of all the difficulties that have appeared in the literature.

The differential operator written above can only be applied to absolutely continuous functions, but there are further requirements. One such is that  $\hat{T}_{AB}\psi$  belongs to  $\mathcal{H}_p$ , i.e., that it be square integrable. This poses a restriction due to the singularity of the operator at  $p = 0$ . On computation, one finds that the singularity is avoided if the function  $\psi$  has one of the following possible behaviours close to  $p \rightarrow 0$ : either  $\psi(p) \sim p^{1/2}$ , or  $\psi(p)/p^{3/2} \rightarrow 0$ . However, this is not enough to fix the domain of the operator, as Paul noticed long ago [9]. Given that, at least formally,  $\hat{T}_{AB}$  is symmetric, this should also be a requirement on its domain. Integration by parts, and demanding that  $\langle \varphi | \hat{T}_{AB} \varphi \rangle$  be equal to  $\langle \hat{T}_{AB} \varphi | \varphi \rangle$  for all  $\varphi$  in the domain of  $\hat{T}_{AB}$ , leads us to exclude the first possibility, thus defining the domain of  $\hat{T}_{AB}$ ,  $D(\hat{T}_{AB})$ , as the set of absolutely continuous square integrable functions of  $p$  on the real line, such that  $\psi(p)/p^{3/2} \rightarrow 0$  as  $p \rightarrow 0$  and  $\|\hat{T}_{AB}\psi\|^2$  is finite. As for the alternative expression  $-i\hbar m p^{-1/2} \partial_p p^{-1/2}$ , let us ask that  $(\Theta(p) - i\Theta(-p))\psi(p)/\sqrt{|p|}$  be absolutely continuous for  $\psi$  to be in its domain. This, together with the further requirement of symmetry, leads us to a domain that coincides with that of  $\hat{T}_{AB}$ . Since the respective actions also coincide over this domain, we see that they are but equivalent differential expressions for the operator, once the adequate domain is taken into account.

$\hat{T}_{AB}$  is closed over this domain, as can be checked by computing  $(\hat{T}_{AB}^\dagger)^\dagger$  (there is no doubt that  $D(\hat{T}_{AB})$  is dense in  $\mathcal{H}_p$ , so the closure of  $\hat{T}_{AB}$  must coincide with  $(\hat{T}_{AB}^\dagger)^\dagger$ ). Before that, though, let us examine  $\hat{T}_{AB}^\dagger$  and its domain.

In order to apply von Neumann's formula, we have to check whether there are states  $\psi$  in  $\mathcal{H}_p$  such that for all  $\varphi \in D(\hat{T}_{AB})$  the following expression holds:

$$\langle \psi | (\hat{T}_{AB} + i) \varphi \rangle = 0,$$

since then  $\psi$  is an eigenvector of  $\hat{T}_{AB}^\dagger$  with eigenvalue  $i$ . Analogously, we also have to study the case with eigenvalue  $-i$ . By integration by parts, and application of the condition that all functions in  $D(\hat{T}_{AB})$  satisfy, namely, that  $\varphi(p)/p^{3/2}$  tends to zero as  $p$  tends to zero, it is found that there are two independent eigenvectors with eigenvalue  $i$ , and none with eigenvalue  $-i$ . The relevant eigenvectors are

$$\psi_\pm(p) = \Theta(\pm p) \sqrt{\mp p} e^{-p^2/2m\hbar}.$$

Notice that, contrary to the expectations of some authors [10,16,17], both of them have to be taken into account: there are no requirements of derivability or continuity for the functions in the domain of the adjoint.

The deficiency indices are therefore  $(2, 0)$ , and we have a maximally symmetric operator. As we have seen in the previous section, this implies that no self-adjoint extension can exist, and we should redo for this case the analysis performed for the momentum operator on the half-line. However, the most convenient way of doing that is by passing to the energy representation, as was already pointed out by Allcock in his seminal work [8], and emphasized again by Kijowski [11,12]. This change of representation is useful, from the mathematical point of view, because it implements a theorem [22] which states that a simple symmetric operator with deficiency indices  $(n, 0)$  can be decomposed as a direct sum of  $n$  operators with deficiency indices  $(1, 0)$ . Since each of these is in fact isomorphic to the momentum operator on the half-line, we will be able to use directly the previous results.

The change of representation corresponds to the decomposition of the Hilbert space  $\mathcal{H}_p$  into the subspaces of positive and negative momentum, i.e.,

$$\begin{aligned} L^2(\mathbf{R}, dp) &= L^2(\mathbf{R}^+, dE) \oplus L^2(\mathbf{R}^+, dE) \\ &= \mathcal{H}_+ \oplus \mathcal{H}_-, \end{aligned}$$

where the first subspace is that of positive momenta, whereas the second corresponds to negative  $p$ . The explicit isomorphism is given by

$$\begin{aligned} \psi_\pm(E) &= (m/2E)^{1/4} \psi(\pm\sqrt{2mE}), \\ \psi(p) &= \left(\frac{|p|}{m}\right)^{1/2} \left[ \Theta(p) \psi_+ \left(\frac{p^2}{2m}\right) + \Theta(-p) \psi_- \left(\frac{p^2}{2m}\right) \right], \end{aligned}$$

where  $\psi \in \mathcal{H}_p$ ,  $\psi_\pm \in \mathcal{H}_\pm$ , and the isomorphism relates  $\psi \leftrightarrow (\psi_+, \psi_-)$ . The factor  $E^{-1/4}$  is due to the change in the measure from  $dp$  to  $dE$  and reciprocally for the factor  $(|p|/m)^{1/2}$ . The interesting point is that given this isomorphism, the time operator of Aharonov and Bohm takes the form  $-i\hbar \partial_E$ , as is well known. The domain of the operator,  $D(\hat{T}_{AB})$  is sent by the isomorphism into the direct sums of square integrable absolutely continuous functions in each subspace, such that for each subspace we have the restriction that  $\psi_\alpha(E)E^{-1/2} \rightarrow 0$  as  $E \rightarrow 0$ . But this is exactly the case considered above, since the requirement  $\psi_\alpha(0) = 0$  and the square integrability

of  $\psi'_\alpha(E)$  imply the restriction stated before. In other words, we have the isomorphism

$$\hat{T}_{AB} = (-i\hbar\partial_E) \oplus (-i\hbar\partial_E) = \hat{T}_+ \oplus \hat{T}_-,$$

where  $\hat{T}_\pm$  are isomorphic to the momentum operator on the half-line.

Therefore, the constructions carried out in the previous section can be immediately translated to this situation, but taking into account that the energy spectrum is degenerate whereas the position spectrum is not. For instance, the complete non-orthogonal set of generalized eigenfunctions  $\psi_p$  is doubled here into a set with a continuous parameter  $t$  (the notation is intended to be suggestive) and a discrete one, with values  $+$  or  $-$ , as follows:

$$\psi_+^{(t)}(E) = \left( \frac{1}{\sqrt{2\pi\hbar}} e^{iEt/\hbar}, 0 \right)$$

and

$$\psi_-^{(t)}(E) = \left( 0, \frac{1}{\sqrt{2\pi\hbar}} e^{iEt/\hbar} \right).$$

In what follows we will not make the explicit distinction between the element of the full Hilbert space and its component, if only one is zero.

These functions transform under the isomorphism to give the following expressions:

$$\tilde{\psi}_\alpha^{(t)}(p) = \Theta(\alpha p) \left( \frac{\alpha p}{2\pi m\hbar} \right)^{1/2} e^{ip^2 t/2m\hbar}.$$

It is straightforward to prove completeness, i.e.,  $\sum_\alpha \int_{-\infty}^{\infty} dt \tilde{\psi}_\alpha^{(t)}(p') \tilde{\psi}_\alpha^{(t)}(p) = \delta(p - p')$ . Alternatively,  $\sum_\alpha \int_{-\infty}^{\infty} dt \psi_\alpha^{(t)}(E') \psi_\alpha^{(t)}(E) = \delta(E - E') \mathbb{1}$ , where  $\mathbb{1}$  is the two by two identity matrix ( $\delta(E - E') \mathbb{1}$  is the identity operator on the full Hilbert space  $\mathcal{H}_+ \oplus \mathcal{H}_-$ ).

Nonorthogonality is also a direct translation:

$$\int_0^\infty dE \psi_{\alpha'}^{(t')}(E) \psi_\alpha^{(t)}(E) = \frac{1}{2} \delta_{\alpha\alpha'} \left( \delta(t - t') + \frac{i}{\pi} \mathcal{P} \frac{1}{t - t'} \right)$$

or

$$\int_{-\infty}^\infty dp \tilde{\psi}_{\alpha'}^{(t')}(p) \tilde{\psi}_\alpha^{(t)}(p) = \frac{1}{2} \delta_{\alpha\alpha'} \left( \delta(t - t') + \frac{i}{\pi} \mathcal{P} \frac{1}{t - t'} \right).$$

It now behooves us to compute the POVM or, alternatively, the probability distribution for measured values of the  $\hat{T}_{AB}$  operator from which it can be readily recovered. By direct translation, we can write the probability density as

$$\Pi_{(\psi_+, \psi_-)}(t) = \left| \int_0^\infty dE \frac{e^{-iEt/\hbar}}{\sqrt{2\pi\hbar}} \psi_+(E) \right|^2 + \left| \int_0^\infty dE \frac{e^{-iEt/\hbar}}{\sqrt{2\pi\hbar}} \psi_-(E) \right|^2,$$

in the energy representation, or as

$$\Pi_\psi(t) = \left| \int_0^\infty dp \left( \frac{p}{2\pi m\hbar} \right)^{1/2} e^{-ip^2 t/2m\hbar} \psi(p) \right|^2 + \left| \int_{-\infty}^0 dp \left( \frac{-p}{2\pi m\hbar} \right)^{1/2} e^{-ip^2 t/2m\hbar} \psi(p) \right|^2,$$

in the momentum representation. This is, of course, the same as Kijowski's probability density. The essential property of covariance under transformations generated by the Hamiltonian is also evident and a direct translation of the covariance property signalled in the previous section. Physically, it means that the probability of arriving at  $t$  for a given state is equal to the probability of arriving at  $t - \tau$  for the same state evolved a time  $\tau$ . This is the reflection on the probability density of the canonical commutation relation  $[\hat{H}, \hat{T}_{AB}] = i\hbar$ .

The domain of  $\hat{T}_{AB}$ , now defined through the POVM, can be characterized as the set of elements of the Hilbert space for which  $\int_{-\infty}^\infty dt \Pi_\psi(t) t^2$  is finite, and this quantity defines  $\langle \hat{T}_{AB} \psi | \hat{T}_{AB} \psi \rangle$  (thus realizing the minimum variance demanded by Kijowski and Werner [11,13]).

As before, we would like to understand all these constructions in terms of a generalized self-adjoint extension, by using the uniqueness of the POVM associated with a maximally symmetric operator, and Naimark's theorem. From the structure of the time operator of Aharonov and Bohm, namely  $\hat{T}_{AB} = (-i\hbar\partial_E) \oplus (-i\hbar\partial_E)$  on  $L^2(\mathbf{R}^+, dE) \oplus L^2(\mathbf{R}^+, dE)$ , it follows that a *natural* and simple extension (natural in the sense of following the natural extension in the analogy) is the operator  $(-i\hbar\partial_E) \oplus (-i\hbar\partial_E)$  acting on  $L^2(\mathbf{R}, dE) \oplus L^2(\mathbf{R}, dE)$ , which is obviously self-adjoint. In other words, we have introduced negative energies, respecting the twofold degeneracy of the initial spectrum. On this space the (doubled) Fourier transform acts as a unitary transformation that provides us with the *time* representation of the states, and the probability density for the time of arrival over a pure state in this extended space is nothing but the modulus squared of the wavefunction in the time representation. Notice that the time representation corresponds to the doubled space  $L^2(\mathbf{R}, dt) \oplus L^2(\mathbf{R}, dt)$ . We reobtain the by now usual probability density for time of arrival, by restriction to the initial Hilbert space. The restrictions to the initial Hilbert space of the applications of the spectral theorem are therefore related to  $\Pi_\psi(t)$ , as stated before.

The problems that the vicinity of  $p = 0$  (alternatively  $E = 0$ ) pose for the analysis of the operator of Aharonov and Bohm are thus seen to be due to the (physically imposed) restriction to the space of positive energies. There is a reminder of the negative energies in aspects such as the nonorthogonality of the set of generalized eigenfunctions, similarly to what happens in the paradigmatic example of the previous section.

#### IV. GENERAL TIME OPERATORS

In previous sections we have discussed the time of arrival for free motion but in fact its mathematical form, and its POVM, can easily be generalized for arbitrary potential functions. The important point however is that in general the resulting operators and POVMs cannot be physically associated with an arrival time.

Consider a self-adjoint Hamiltonian, bounded from below, defined on a Hilbert space  $\mathcal{H}$ , such that the spectral decomposition leads to the isomorphism

$$\mathcal{H} = \oplus_{i=1}^N \left( \oplus_{j=1}^{n_i} L^2([a_i, \infty), d\mu_i(E)) \right),$$

where all the measures  $\mu_i$  are absolutely continuous with respect to the Lebesgue measure. That is to say, the spectrum of the Hamiltonian is absolutely continuous, and for any given  $E \in \mathbf{R}$  the degeneracy is finite, the maximum degeneracy being  $\sum_{i=1}^N n_i$ . The Hamiltonian is realized in each subspace as the multiplication by the variable  $E$ . Therefore, a natural (but most definitely not unique) candidate for the time operator is again  $-i\hbar\partial_E$  on each of these subspaces, restricted to functions that vanish at  $a_i$ . Again each component of this time operator can be extended to the real line, where it will be self-adjoint and admit a spectral decomposition, which, by projection, will give us again the POVM associated with our candidate operator. The POVM, and its associated probability density, will be unique for the given operator if this is indeed maximally symmetric.

Notice moreover that if we do extend one of the Hilbert subspaces to be square  $\mu$ -integrable functions on the real line, and demand that the covariance property of the restriction of the time operator to that Hilbert subspace be maintained on the real line, then, under fairly general conditions, the extension of time operator and Hamiltonian on  $L^2(\mathbf{R}, d\mu_i(E))$  will be unitarily equivalent to the canonically conjugate pair  $-i\hbar\partial_E$  and multiplication by  $E$ . Therefore, modulo intervening unitary transformations, we have a way of constructing POVMs for time operators by Naimark dilations.

The usefulness or otherwise of the particular time operator under consideration will then have more to do with its actual properties and measured probability density rather than with mathematical difficulties that had riddled the work of many previous workers in the field.

To illustrate this point further, let us examine the standard example of a particle in a constant field. The Hamiltonian is  $\hat{H}_g = \hat{p}^2/2m + mg\hat{q}$ , clearly seen to be unbounded. Pauli's argument is therefore not applicable, and a self-adjoint operator canonically conjugate to  $\hat{H}_g$  does indeed exist, namely,  $\hat{T}_g = \hat{p}/mg$ . In the energy representation this operator is of course given by  $-i\hbar\partial_E$ . It can be ascribed to time of arrival to zero momentum, but in no possible way to time of arrival to a specified position. This example tells us that an operator having the form  $-i\hbar\partial_E$  in the energy representation, be it as a self-adjoint operator, or associated with a POVM, does

not necessarily mean that we have obtained a time-of-arrival operator, even though a time operator is indeed being considered.

At this point it is worthwhile mentioning the approach of León et al. [25], intended to generalize  $\hat{T}_{AB}$  to the interacting case of a potential barrier (under the hypothesis of asymptotic completeness and absence of bound states). They do obtain good time operators, involving  $-i\hbar\partial_E$  in the basis of outgoing or incoming scattering states, and their distributions, understood as POVMs. However, since the expectation value of these operators is, over a given state, the same as the expected time of arrival that the corresponding asymptotic states (outgoing or incoming respectively) would produce in the case of no interaction, it is hard to understand them as bona fide time-of-arrival operators at an arbitrary spatial point.

Finally, it is also interesting to examine the relation of the operator  $\hat{T}_{AB}$  with older literature on the "time operator" by Olkhovski, Recami, and others [26]. The basic idea behind this set of works is to extract a time operator from the relation that defines an average "presence time" at  $x = 0$  by

$$\langle t \rangle \equiv \frac{\int_{-\infty}^{+\infty} dt |\psi(x=0, t)|^2 t}{\int_{-\infty}^{+\infty} dt |\psi(x=0, t)|^2}.$$

We shall discuss as in [26] the simple case of states without negative momenta so that there is no need to consider the energy degeneracy in the following expressions. The energy Fourier transform of  $\psi(x=0, t)$  is given by

$$\begin{aligned} \eta(E) &= h^{-1/2} \int_{-\infty}^{+\infty} \psi(x=0, t) e^{iEt/\hbar} dt \\ &= h^{1/2} \langle x=0 | E \rangle \langle E | \psi(t=0) \rangle. \end{aligned}$$

In terms of  $\eta$  we can write

$$\langle t \rangle = -i\hbar \int_0^\infty dE \tilde{\eta}(E)^* \frac{\partial \tilde{\eta}(E)}{\partial E},$$

where  $\tilde{\eta}(E) \equiv \eta(E)/(\int dt |\psi(0, t)|^2)^{1/2}$ . Thus a "time operator" may be again identified with  $-i\hbar\partial_E$ , but now in the space of functions  $\tilde{\eta}(E)$ . This operator is different from  $\hat{T}_{AB}$ .

In terms of the position and momentum operators the average presence time becomes

$$\langle t \rangle = -\frac{m}{2} \frac{\langle \psi(t=0) | \hat{p}^{-2} \hat{x} + \hat{x} \hat{p}^{-2} | \psi(t=0) \rangle}{\langle \psi(t=0) | \hat{p}^{-1} | \psi(t=0) \rangle}, \quad (1)$$

provided the integrals exist. This is to be contrasted with the average time that can be defined using the current density  $J(x=0, t)$ ,

$$\langle t \rangle_J \equiv \frac{\int_{-\infty}^\infty dt J(x=0, t)}{\int_{-\infty}^\infty dt J(x=0, t)} = \langle \psi(t=0) | \hat{T}_{AB} | \psi(t=0) \rangle. \quad (2)$$

The different formal results are to be expected since, in the classical limit, (1) is associated with an average presence time and (2) with an average passage time. Note however that in both cases we can relate these measurements with the formal operator  $-i\hbar\partial_E$ , as has been pointed out all along.

As stated above, no matter how one constructs general time operators, one is inevitably led to  $-i\hbar\partial_E$  (plus, possibly, a function of  $E$ ), but the physical interpretation of those operators, self-adjoint or associated with a POVM, is quite another issue.

## V. DISCUSSION

In the sections above we have made reference to results and proposals of other workers in the subject. In this section, however, we intend to restate some of those results and discussions in the light of our description. To start with, none better than the initial paper of Aharonov and Bohm [7], where they introduce the operator  $\hat{T}_{AB}$ . They were not particularly concerned with the self-adjointness or otherwise of the operator, but they did signal the problem of the singularity for  $p = 0$ , which they brushed aside by stating that all components of the interesting wavefunctions would be of high enough momentum. Insofar as that is the case, then there is indeed no problem in obtaining a probability distribution for measurements of the operator. Their real point of interest in introducing  $\hat{T}_{AB}$  was to show that there is no reason inherent in the principles of quantum mechanics for the energy of an observed system not to be observed in as short a time as one pleases, where the time is measured in an observer system. The topic of measurement limitations is retaken in much later work of Aharonov and others [27], where they make the distinction between direct and indirect measurements of time of arrival, indirect measurements being associated with  $\hat{T}_{AB}$  (or with regularized variants), and direct measurements with couplings of the particle with other degrees of freedom that in the classical limit would measure the time of arrival. They describe a lower bound for the time uncertainty of direct measurements inversely proportional to the typical energy of the particle (not to the energy uncertainty). In fact the same dependence has been recently described, and traced back to the lower bound of the energy spectrum, for the indirect measurement case [28]. But the time uncertainty refers to an ensemble and does not preclude a precise determination of the time of arrival in an individual measurement, in other words, this does not involve a limitation of the quantum theory to handle the arrival time concept and prescribe *intrinsic* arrival time distributions (formulated without explicit recourse to a measuring apparatus or an additional “clock” degree of freedom). Numerical results have shown essential agreement between the (intrinsic) POVM distribution and operational distributions given by phenomenological screen models, except

in rather pathological cases [29,30].

Going back in time again, we come to the work of Allcock [8]. As we have signalled above, he advocated the use of the energy representation. Even more, he signalled the need for negative energies in a particular way. If we indeed want to measure arrival times, we would have to prepare wavepackets that are localized on one side of the point of arrival ( $x = x_0$ , say) for all times before a given one,  $t < t_0$ . This directly entails that the temporal Fourier transform of the wavefunction will exhibit all positive and negative energies, save for a set of null measure. In a way, it could be argued that the conceptual setup for measuring time of arrival requires by itself the introduction of negative energies. Furthermore, the proof he proposes for the need for all positive and negative energies is also illuminating: it goes the way of the Paley-Wiener-Titchmarsh theorem and the uniqueness theorem for analytic continuations. This is precisely the same route taken to show the non-orthogonality of any set of functions that could be considered as (generalized) eigenfunctions of a time operator. In that proof it is clear that the introduction of negative energies also eliminates the problem of non-orthogonality. However, his interpretation of the non-orthogonality of (generalized) eigenfunctions for the time of arrival as precluding any measurement thereof is at odds with the operational approach within which the POVM idea takes place.

A number of more mathematical papers has also been published, with a more functional analytical approach than those mentioned before [9,10,14].

The axiomatic approach of Kijowski [11] has been mentioned all along, since its guiding idea, i.e., characterizing the physical content of a concept such as time of arrival in a probability distribution, is crucial for our purposes, and clears the path for the introduction of the POVM as the physically relevant object. Kijowski also emphasized the usefulness of the energy representation, and decomposed the Hilbert space of the free particle as the direct sum of the subspaces of positive and negative momenta. He constructs both the operators  $\hat{T}_{\pm}$  (in his notation,  $\hat{t}_{\pm}^Q$ , if  $Q$  is the point  $x_3 = 0$ ) by comparison with the probability distribution, as we do. He then points out that  $\hat{T}_{+} \oplus \hat{T}_{-}$  admits no self-adjoint extension, and goes no further that way. However, he also introduces a particularly interesting object, retaken more recently by Delgado and Muga [15] (see also [12]), namely  $\hat{T}' = \hat{T}_{+} \oplus (-\hat{T}_{-})$ . He then asserts that this operator is essentially self-adjoint. Let us examine this question from the point of view taken in this paper. As we have signalled, both  $\hat{T}_{+}$  and  $\hat{T}_{-}$  are isomorphic to the momentum operator on the half-line, and their deficiency indices are  $(1, 0)$  for both of them. Therefore,  $-\hat{T}_{-}$  is also a maximally symmetric operator, with deficiency indices  $(0, 1)$ . The total operator  $\hat{T}_{+} \oplus (-\hat{T}_{-})$ , symmetric on a dense subspace, has deficiency indices  $(1, 1)$ , so it is not self-adjoint, although it admits self-adjoint extensions. Contrary to what might be inferred



from some claims in [12], there are infinite self-adjoint extensions, parametrized by  $\alpha \in [0, 2\pi)$ . The extension  $\hat{T}'_\alpha$  is defined on  $D(\hat{T}'_\alpha)$ , which is the set of elements of  $\mathcal{H}_+ \oplus \mathcal{H}_-$  of the form  $(\psi_+ + \lambda e^{-E/\hbar}, \psi_- + \lambda e^{i\alpha} e^{-E/\hbar})$ , where  $\psi_\pm \in D(\hat{T}_\pm)$ , and  $\lambda \in \mathbb{C}$ . The action on its domain is simply that of the couple of differential operators  $(-i\hbar\partial_E, i\hbar\partial_E)$ . The boundary conditions, however, are different. In terms of the momentum representation, the functions in the domain of  $\hat{T}'_\alpha$  can have  $p^{1/2}$  behaviour, for instance. At any rate, the probability distribution deduced from these operators is not covariant under time shifts, so their physical interpretation is rather clouded unless the state belongs to only one of the two subspaces (positive or negative momenta) [20].

Another interesting attempt to construct a self-adjoint operator related to the time of arrival is that of Grot, Rovelli and Tate [16]. In essence, they give a realization of the intuition of Aharonov and Bohm [7] that for high momenta the  $p = 0$  singularity of the differential operator is irrelevant, a point later taken up by Paul [9] as well. However, this generalized self-adjoint operator has also some drawbacks from the point of view of its interpretation [20,17]. From the point of view taken in this paper, the problem with the proposal of Grot, Rovelli and Tate is that the strong operator limit of their deformed operator does not exist when their regulator is made to disappear (this can be seen, for example, computing the norm of the action by the regulated operator on any gaussian state, and then trying to eliminate the regulator - the norm blows up). Therefore, the results obtained with the regulator cannot be at all extrapolated to the unregulated case.

Closest to the work carried out in this paper is the presentation by Busch, Grabowski and Lahti [5,6]. However, they refer the idea of using Naimark's dilation in this context to the paper of Werner [13], where he constructs "screen observables" using a version of imprimitivity adequate for the case of POVMs. Our analysis is much more simplified and explicit.

In conclusion, we have given a description of the POVMs associated with the momentum operator on the half-line and the time operator of Aharonov and Bohm in terms of Naimark's dilations. More concretely, in terms of what for the momentum operator is the natural dilation. We have clarified several issues that have been the matter of debate or confusion in the literature as of late, in particular the deficiency indices and constructions of self-adjoint extensions of  $\hat{T}_{AB}$ , and we have rederived the probability density for times-of-arrival derived axiomatically by Kijowski. We have also made a proposal for the construction of the probability distributions of a wide class of time operators, for which it has been shown that they are not in general related to the arrival time, in spite of the formal agreement with the arrival time operator of the free motion case.

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